Indian J. Phys. 77A (2), 167–171 (2003)

AN INTERNATIONAL JOURNAL IJPA

Theoretical study of superconducting gap in correlated cuprates

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Abstract : The interplay between superconductivity (SC) and anti-ferromagnetism (AF) in strongly correlated High Temperature Superconductor systems : $R_{2-x}M_xCuO_4$ (R = Nd, La, .. and M = Sr, Ce) is very interesting to study both theoretically and experimentally. We present a microscopic theoretical model for the system to study its superconducting gap equations in absence of anti-ferromagnetism. Superconductivity is assumed to be in copper $3d$ electrons in presence of hybridization between conduction band and f-level of the Ce impurity atom. Green's functions are calculated by Zubarev technique and the SC gap equation was solved numerically by self-consistent method under half-filled band situation. The effect of the impurity f-level and its hybridization with conduction band on superconducting gap is investigated theoretically and results are discussed in this communication.

Keywords : Magnetic superconductors, antiferromagnetic order, Cu-O planes.

PACS Nos. : 74.72.–h, 71.38.–h, 75.50.Ee

1. Introduction

The $R_{2-x}M_xCuO_4$ compounds (R = rare-earth and M = Ce, Th, Sr, Ba, ...) have intensively studied soon after their discovery. For R = Pr, Nd, Sm, Eu and x = 0.15, n-type superconductivity is achieved after appropriate thermal treatment in reduced atmosphere [1], but compounds with R = Gd to Tm are not superconductors for any doping concentrations [2]. In R_2CuO_4, the copper moments order anti-ferromagnetically below $T_N \simeq 240 - 280$ K [3]. For heavier R these compounds show weak ferro-magnetism (WFM), with a boundary at R = Eu [4]. For R = Tb, Dy, Ho, Dr, Tm and Y, the T'-type structure can be synthesized only under high pressure, with again a boundary for structural stability at the center of R-series [5]. The hole doped $La_{2-x}Sr_xCuO_4$ system shows superconductivity for fairly wide range of doping, $0.005 \le x \le 0.25$ [6]. Besides, superconductivity has not been observed for $Gd_{2-x}Ce_xCuO_4$ for $0 \le x \le 0.15$. It remains puzzling that many cuprates with familiar CuO_2 planes are not superconducting [7–9], although it is established that the CuO_2 planes play an important role in superconductivity of cuprates. The study of such cuprates is of particular interest because it is likely to offer important clues to the behaviour of their superconducting counter parts. This motivates us to carry out a systematic theoretical study. Out of the several high-T_c superconductors, ($R_{2-x}M_xCuO_4$) (R = Nd, Pr, ..., M = Sr, Ce, ...) compounds have received a considerable amount of attention soon after their discovery, because they become electron carrier superconductors. When Nd_2CuO_4 is doped with Ce impurity it changes its insulating phase to the semi-conducting phase with Ce concentration $x \sim 0.10$. The extra electron of Ce enters into CuO_2 plane and gives rise to superconductivity at $x = 0.15$. This superconducting phase co-exists with anti-ferromagnetic (AFM) ordering. We report here a microscopic model to study the temperature dependence of superconducting gap of the high temperature superconductor in absence of magnetism.

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2. Formalism

The non-magnetic ground state of the electron doped system $Nd_{2-x}Ce_xCuO_4$ [NCCO] is described below. The conduction electron Hamiltonian is given by

$$H_c = \sum_{k,\sigma} \epsilon_0(k) \left(a^\dagger_{k,\sigma} b_{k,\sigma} + b^\dagger_{k,\sigma} a_{k,\sigma} \right). \tag{1}$$

Here $a^\dagger_{k,\sigma}$ and $b^\dagger_{k,\sigma}$ are the creation operators of electrons at sites 1 and 2 of copper respectively. Two sub-lattices of the conduction electrons are assumed to introduce anti-ferromagnetism (AFM) in future models. The hopping takes place between neighbouring sites of copper with dispersion $\epsilon_0(k) = -2t_0(\cos k_x + \cos k_y)$. The Hamiltonian

$$H_f = \epsilon_f \sum_{k,\sigma} \left(f^\dagger_{1,k,\sigma} f_{1,k,\sigma} + f^\dagger_{2,k,\sigma} f_{2,k,\sigma} \right) \tag{2}$$

is the intra f-electron Hamiltonian and $\hat{\epsilon}_f$ is the renormalized f-level energy corresponding to two sub-lattices 1 and 2.

When the material is doped, the charge carriers enter the CuO_2 plane and destroy the long range AFM order. Depending on the concentration of the doping and the temperature range, a complex disordered phase is formed in the CuO_2 plane. This disorder phase can be represented by the on-site f-level energy of the non-magnetic impurity rare-earth ion (Ce) in NCCO and the hybridization between f-level and the Cu-3d electron bands. The Hamiltonian

$$H_v = V \sum_{k,\sigma} \left\{ \left(a^\dagger_{k,\sigma} f_{1,k,\sigma} + b^\dagger_{k,\sigma} f_{2,k,\sigma} \right) + h.c \right\} \tag{3}$$

is the effective hybridization between the f-electrons of the rare-earth ions and the conduction electrons of copper 3d-electrons. H_I describes the attractive interaction of the charge carriers in the Cu–O planes leading to Cooper pair formation. Here BCS type weak coupling Cooper pairing of conduction electrons of two different copper sites is taken into account. The superconducting state of the system is described by the interaction Hamiltonian H_I.

$$H_I = -\Delta \sum \left[a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} + b^\dagger_{k\uparrow} b^\dagger_{-k\downarrow} + h.c \right]. \tag{4}$$

Here D is the superconducting gap parameter. The total Hamiltonian is written as

$$H = H_c + H_f + H_v + H_I. \tag{5}$$

3. Calculation of super-conducting gap

We calculate one electron Green function using the Hamiltonian H given in eq. (5) for the superconducting state of the cuprate system. The double time electron Green function of Zubarev type [10] are calculated by equations of motion method. The Green functions involved in the calculation are defined as

$$A_1(k,w) = \left\langle\left\langle a_{k,\uparrow} ; a^\dagger_{k,\uparrow} \right\rangle\right\rangle_w ;$$

$$A_2(k,w) = \left\langle\left\langle a^\dagger_{-k,\downarrow} ; a^\dagger_{k,\uparrow} \right\rangle\right\rangle_w ;$$

$$B_1(k,w) = \left\langle\left\langle b_{k,\uparrow} ; b^\dagger_{k,\uparrow} \right\rangle\right\rangle_w ;$$

$$B_2(k,w) = \left\langle\left\langle b^\dagger_{-k,\downarrow} ; b^\dagger_{k,\uparrow} \right\rangle\right\rangle_w .$$

The coupled equations involving the above Green functions are solved to find out $A_{1,2}(k,w)$ as

$$A_1 = (\omega - \epsilon_f) \frac{(\omega + \epsilon_0)(\omega + \epsilon_f) - V^2}{4\pi |D_1(\omega)|}$$

$$\frac{(\omega - \epsilon_0)(\omega + \epsilon_f) - V^2}{4\pi |D_2(\omega)|} \tag{6}$$

$$A_2 = -\frac{\Delta(\omega^2 - \epsilon_f^2)}{4\pi} \left[\frac{1}{|D_1(\omega)|} ' |D_2(\omega)| \right. \tag{7}$$

where $|D_1(\omega)| = \omega^4 - S_1\omega^2 + T_1$

and $|D_2(\omega)| = \omega^4 - S_1\omega^2 + T_2$

with $E_k^2 = \left(\epsilon_0^2(k) + \Delta^2 \right)$. (8)

The poles of the Green functions $A_1(k,w)$ and $A_2(k,w)$ give eight quasi-particle energy bands which are given by

$$\pm\omega_{1,2} = \tag{9}$$

$$\pm\omega_{3,4} = \left|\left| \frac{S_1 \pm \sqrt{S_1^2 - 4T_2}}{2} \right.\right. \tag{10}$$

where $S_1 = E_k^2 + \epsilon_f^2 + 2V^2$,

$T_1 = E_k^2 \epsilon_f^2 - 2V^2 \epsilon_f \epsilon_0 + V^4$,

and $T_2 = E_k^2 \epsilon_f^2 + 2V^2 \epsilon_f \epsilon_0 + V^4$. (11)

The superconducting gap is defined as

D = D[1] + D[2]

where $\Delta^1 = -\sum_k \bar{V}_k \left\langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} \right\rangle$

and $\Delta^2 = -\sum_k \bar{V}_k \left\langle b^\dagger_{k\uparrow} b^\dagger_{-k\downarrow} \right\rangle$. (12)

The final expression for superconducting energy gap is

$$\Delta = V_0 N(0) \int_{-\omega D}^{+\omega D} d\epsilon_0(k) \left[\frac{F_1}{\omega_1^2 - \omega_2^2} + \frac{F_2}{\omega_3^2 - \omega_4^2} \right], \quad (13)$$

where $F_1 = F_{11}(\epsilon_0(k), T) - F_{12}(\epsilon_0(k), T)$,

and $F_2 = F_{13}(\epsilon_0(k), T) - F_{14}(\epsilon_0(k), T)$

with $$F_{1i}(\epsilon_0(k), T) = \frac{\omega_i^2 - \epsilon_f^2}{\omega_i} \tan h \frac{\beta \omega_i}{2} \quad (14)$$

for $i = 1$ to 4. $N(0)$ is the density of states of the conduction electrons at the Fermi level ϵ_F and V_0 is effective coupling potential. Different quantities involved are made dimensionless dividing them by the hopping integral $2t_0$. $W = 8t_0$ is the width of the conduction band. The dimensionless parameters are given by

$$\frac{\Delta}{2t_0} = z; \quad \frac{\omega_D}{2t_0} = \tilde{\omega}_D; \quad \frac{K_B T}{2t_0} = t;$$

$$\frac{V}{2t_0} = v; \quad \frac{\epsilon_0(k)}{2t_0} = x_0; \quad N(0)V_0 = g.$$

The superconducting gap equation in dimensionless form

$$z = g \int_{-\tilde{\omega}_D}^{+\tilde{\omega}_D} dx_0 \left[\frac{1}{\tilde{\omega}_1^2 - \tilde{\omega}_2^2} \{F_{11}(x_0, t) - F_{12}(x_0, t)\} + \frac{1}{\tilde{\omega}_3^2 - \tilde{\omega}_4^2} \{F_{13}(x_0, t) - F_{14}(x_0, t)\} \right], \quad (15)$$

where $F_{1i}(x_0, t) = \frac{\tilde{\omega}_i^2 - d^2}{\tilde{\omega}_i} \tan h \left(\frac{\beta \omega_i}{2} \right)$

and $i = 1$ to 4.

4. Result and discussion

It is seen from the gap equation (15) that the superconducting gap (z) is a function of itself as well as chemical potential describing the temperature dependence of the superconducting gap. So the gap equation is solved self-consistently under half-filling band situation with the Fermi-level lying at the middle of the conduction band. The Fermi-level is taken as zero ($\epsilon_F = 0$). The different reduced parameters involved in the numerical calculations are the superconducting coupling parameter g, superconducting gap z, f-level position d, hybridization strength v and temperature t. Here we have taken the conduction band width $W = 8t_0 \approx 1$eV and the Debye frequency ($\omega_D \approx 250$ K) for high temperature superconductor.

In absence of the f-level position and the hybridization between conduction band and the f-level, the gap equation reduces to BCS gap. Hence, we keep the superconducting coupling $g = 0.2059$ with $d = 0$, $v = 0$ to get the BCS value of superconducting gap at 0 K as $z(0) = 0.0176$ and the superconducting transition temperature $t_c = 0.01$ corresponding to $T_c = 25$ K for high temperature superconductor NCCO. Figure 1 shows the temperature variation of the superconducting gap for various values of

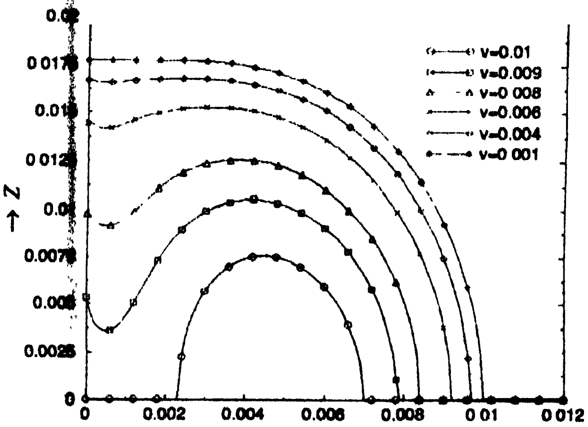

Figure 1. Plot of z vs t for different values of v = 0.001, 0.004, 0.006, 0.008, 0.009, 0.010 and for fixed values of d = 0.001 and g = 0.2059.

hybridization strength v. It is observed that the BCS behaviour in the gap is retained upto a minimum hybridization strength of $v = 0.001$. As hybridization strength v between conduction band and f-level increases from $v = 0.001$ to 0.01, there is suppression of Cooper pairing throughout the temperature range upto transition temperature t_c indicated by the decrease in the superconducting gap parameter z. It is also observed that the increase in hybridization strength causes a decrease in superconducting transition temperature t_c. For stronger hybridization (for $v = 0.01$) the transition temperature decreases substantially giving rise to $t_{c1} = 0.007$ and another $t_{c2} = 0.0024$ at low temperature below which there exists only normal phase upto $t = 0$. Superconductivity exists only within narrow range of temperature from t_{c1} to t_{c2}. Another interesting effect of hybridization is that the gap decreases monotonically to give a maximum dip in z and then increases towards the temperature $t = 0$. This anomalous behaviour of superconducting gap in presence of different hybridization strengths can be explained on the basis of the induced superconducting pairing amplitudes of the type : mixed pairing $\phi^{af} = \langle a_{k,\uparrow} f_{-k,\downarrow} \rangle$, $\phi^{bf} = \langle b_{k,\uparrow} f_{-k,\downarrow} \rangle$ and f-level pairing $\phi^f = \langle f_{k,\uparrow} f_{-k,\downarrow} \rangle$.

Figure 2 shows the plot of z vs t for different values of the f-level position from $d = 0.00001$ to $d = 0.1$. It is observed that if the f-level lies below or above the Fermi-level upto the position $d = \pm 0.00001$ then the BCS behaviour of z remains unaltered. When $d = \pm 0.001$, then BCS behaviour of z is retained but z is reduced from 0.0176 to 0.016 accompanied by a reduction in transition temperature t_c.

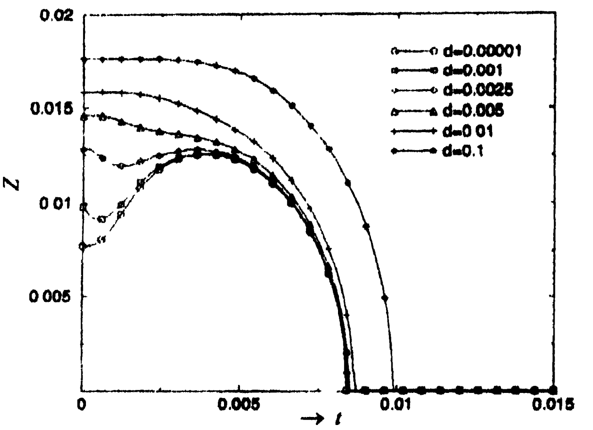

Figure 2. Plot of z *vs* t for different values of d = 0.10, 0.01, 0.005, 0.0025, 0.001, 0.00001 and for fixed values of v = 0.008 and g = 0.2059.

It is observed from the plot that the superconducting transition temperature t_c nearly remains constant as f-level moves away on either side from the Fermi-level. However, the SC gap monotonically decreases, reaches dip and again increases towards lower temperature as f-level moves further away from the Fermi-level. This anomalous behaviour of the SC gap at low temperatures in intricately related to the mixed pairing amplitude ϕ^{af}, ϕ^{bf} and the f-level pairing amplitude ϕ^{f} and the average occupation numbers like n^a, n^b, n^{ab}, n^{af}, n^{bf}. The temperature variation of these quantities will explain the anomaly clearly. This investigation is beyond the scope of this present communication.

Figure 3 shows the z *vs* t plot for various values of the SC coupling constant $g = 0.20$ to $g = 0.24$. For fixed values of the f-level and hybridization, the superconducting gap z and transition temperature t_c are enhanced with the increase of the coupling constant g. However we can not increase g arbitrarily as it is connected with the maximum cutoff Debye frequency ω_D of the phonon mediated superconductivity. It

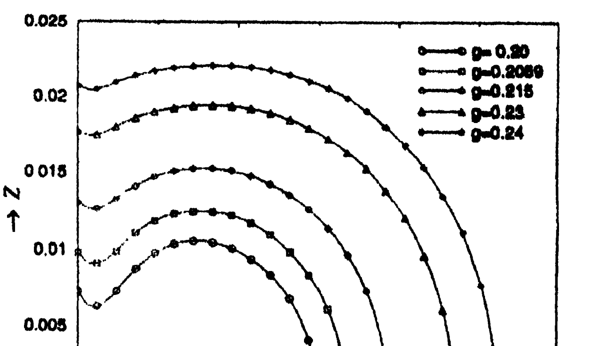

Figure 3. Plot of z *vs* t for different values of g = 0.24, 0.23, 0.215, 0.2059, 0.20 and for fixed values of d = 0.001 and v = 0.008.

is again observed that the SC gap exhibits a dip structure at low temperatures for smaller values of coupling g.

Figure 4 shows the variation of SC gap z with the hybridization v between the conduction and the f-level for fixed values of the temperature and the coupling constant. The increase in hybridization results in monotonic decrease of superconducting pairing for a particular higher strength of the hybridization where the SC pairing completely vanishes. But at low temperatures the SC gap exhibits anomalous behaviour for all possible values of hybridization. The SC gap in the low temperature region needs further investigation.

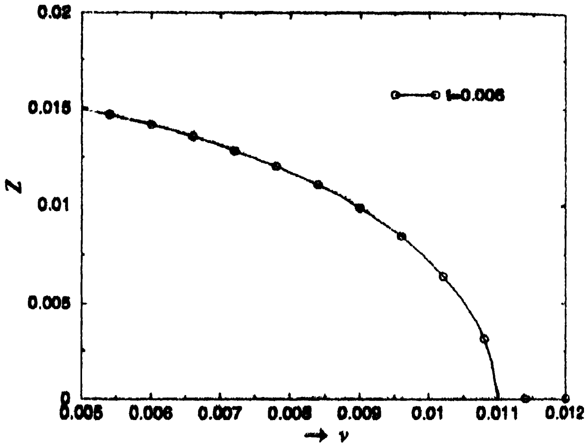

Figure 4. Plot of z *vs* v for fixed values of t = 0.006, d = 0.0025 and g = 0.05835.

Figure 5 shows the plot of z *vs* d for different temperatures. For a fixed value of hybridization v (= 0.008), the SC gap z shows anomaly at low temperatures. As temperature increases from t = 0 to t = 0.004, the SC gap height increases continuously as f-level (d) is moved away from the Fermi-level on either side. As the temperature further increases from t = 0.004, the SC gap z shows a turning point and decreases for all positions of the f-level

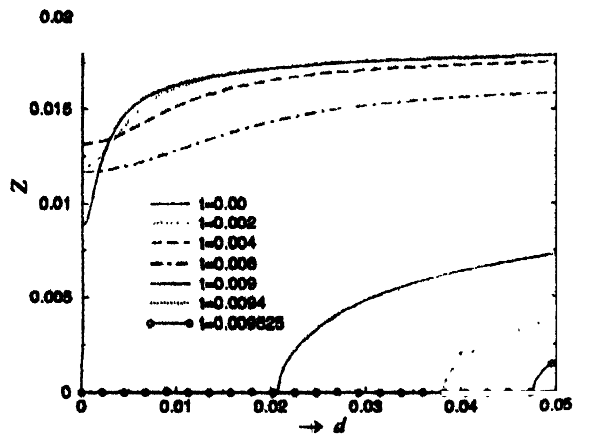

Figure 5. Plot of z *vs* d for different values of t = 0.00, 0.002, 0.004, 0.006, 0.009, 0.0094, 0.009525 and for fixed values of v = 0.008 and g = 0.05835.

away from Fermi-level. As temperature further increases SC gap decreases and vanishes as the f-level is far away from the Fermi-level. The temperature $t^* = 0.004$ below which the SC gap shows anomaly is a temperature scale of the ~ 1 K. This temperature t^* = corresponds to a fluctuation temperature related to the hybridization between the conduction band and the f-level.

Figure 6 shows the plot of z *vs* g for two different temperatures. The SC gap $z(0)$ at $t = 0$ increases linearly.

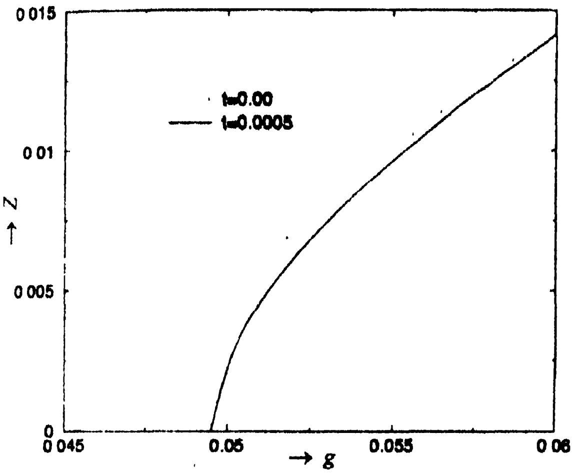

Figure 6. Plot of z *vs* g for t = 0.0, 0.0005 and fixed values of v = 0.008 and d = 0.0025.

The SC gap $z(t)$ at any other finite temperature shows a linear dependence on g for higher SC compling strengths, but SC gap vanishes for lower coupling constants exhibiting a parabolic dependence of SC gap on the coupling constant g. Hence, the low temperature and low coupling dependence of SC gap need further investigation.

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